Spectral shooting is Schubert calculus

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Abstract. We are attempting to show that Schubert cycles, and in particular, special Schubert cycles underpin linear spectral parameter space. First we review Riccati flows on the Grassmannian and introduce a new shifted Riccati flow using Schur complements. Second we consider the tautological spectral sphere bundle and explain how it can be punctured by Schubert cycles. We then suggest some new numerical approaches to spectral location using this idea. Thirdly we consider a practical example that was driven by, but at the same time has also helped conceive, some of the theory/ideas above.

1. Riccati flows

1.1. Projection of linear Stiefel flows. Suppose we are given a linear non-autonomous vector field $V(x,Y)=A(x)\,Y$ for $(x,Y)\in\mathbb{R}\times\mathbb{V}(n,k)$, where $\mathbb{V}(n,k)$ is the Stiefel manifold of k-frames in $\mathbb{C}^n$ centred at the origin. Projecting this flow onto a chosen coordinate patch $\mathbb{U}_{\mathbf{i}}\subset\mathrm{Gr}(n,k)$ of the Grassmannian identified by $\mathbf{i}$, we obtain the following Riccati flow in the coordinate chart variables $\hat{y}\in\mathbb{C}^{(n-k)\times k}$:

$$\hat{y}'=c(x)+d(x)\hat{y}-\hat{y}a(x)-\hat{y}b(x)\hat{y},$$

where a, b, c and d denote the $\mathbf{i}\times\mathbf{i}$, $\mathbf{i}\times\mathbf{i}^\circ$, $\mathbf{i}^\circ\times\mathbf{i}$ and $\mathbf{i}^\circ\times\mathbf{i}^\circ$ submatrices of A, respectively. Here we can think of decomposing $Y=y_{\mathbf{i}^\circ}u$, where $u\in\mathrm{GL}(k)$ is a given rank k submatrix of $Y\in\mathbb{V}(n,k)\cong\mathbb{C}^{n\times k}$, and $y_{\mathbf{i}^\circ}$ is a matrix whose $\mathbf{i}$th rows are the identity matrix and whose remaining rows can be identified with the local coordinate chart variables.

1.2. Spectral matching. Consider the linear spectral problem on $\mathbb{R}$:

$$Y'=A(x;\lambda)\,Y$$

We assume there exists a subdomain $\Omega\subseteq\mathbb{C}$ containing the right-half complex plane, such that for $\lambda\in\Omega$ there exists exponential dichotomies on $\mathbb{R}^-$ and $\mathbb{R}^+$ with the same Morse index k in each case. Let $Y^-(x;\lambda)\in\mathbb{V}(n,k)$ denote the matrix whose columns are solutions to the spectral problem and which span the unstable manifold section at $x\in[-\infty,+\infty)$. Let $Y^+(x;\lambda)\in\mathbb{V}(n,n-k)$ denote the matrix whose columns are the solutions which span the stable manifold section at $x\in(-\infty,+\infty]$.

The values of spectral parameter $\lambda\in\Omega$ for which the columns of Y^- and columns of Y^+ are linearly dependent on $\mathbb{R}$ are isolated pure-point eigenvalues. The *Evans function* $D(\lambda)$ is the measure of the degree linear dependence between the two basis sets Y^- and Y^+, i.e. of the degree of transversal intersection between the unstable and stable manifolds (see Alexander, Gardner and Jones [**1**]):

$$D(\lambda) := \mathrm{e}^{-\int_0^x \mathrm{Tr} A(\xi;\lambda)\,\mathrm{d}\xi} \det\bigl(Y^-(x;\lambda)\ Y^+(x;\lambda)\bigr).$$

It is analytic in Ω. In practice we drop the non-zero, scalar exponential prefactor and evaluate the Evans function at a matching point x_*.

1.3. Modified Riccati flows. Practical integration along the Grassmannian means that the evaluation point x_* can be any real value; we might as well take $x_* = +\infty$. With this in mind we shall define a matching function as follows. Let us fix a flag, for the moment let us use the opposite flag $\mathbb{E}'_\bullet$, and study the linear Stiefel flow projected on the Grassmannian; and in particular how it might percolate through the disjoint cell decomposition of $\mathrm{Gr}(n,k)$. The top cell in this instance is

$$\begin{pmatrix} I_k \\ y \end{pmatrix} \qquad \Leftrightarrow \qquad \begin{pmatrix} I_k & \tilde{y} \end{pmatrix}.$$

To match with the more usual row spanning notation for subspace representation, we will take the top cell to have the representation shown on the right. Note that we use $\tilde{a}$ to denote the transpose of a. We know that y satisfies the Riccati equation $y' = c + dy - ya - yby$; for the top cell with respect to $\mathbb{E}'_\bullet$ we have $\mathbf{i} = \{1,\ldots,k\}$. Hence $\tilde{y}$ satisfies

$$\tilde{y}' = \tilde{c} + \tilde{y}\tilde{d} - \tilde{a}\tilde{y} - \tilde{y}\tilde{b}\tilde{y}.$$

For the integration from left to right we use the opposite flag $\mathbb{E}'_\bullet$. For the far-field data at $x = +\infty$, we use the standard flag $\mathbb{E}_\bullet$. If $B(\lambda) := \tilde{y}^+(+\infty;\lambda)$, we define the *matching matrix* to be

$$\begin{pmatrix} I_k & \tilde{y}(x;\lambda) \\ B(\lambda) & I_{n-k} \end{pmatrix} = \begin{pmatrix} I_k - \tilde{y}(x;\lambda)B(\lambda) & \tilde{y}(x;\lambda) \\ O & I_{n-k} \end{pmatrix} \begin{pmatrix} I_k & O \\ -B(\lambda) & I_{n-k} \end{pmatrix}^{-1}.$$

Since the *matching condition* is the determinant of this matrix, we are motivated to define

$$\hat{y}(x;\lambda) := \tilde{y}(x;\lambda)B(\lambda) - I_k,$$

which is minus the Schur complement of I_{n-k} within the matching matrix; see Meyer [**13**, p. 475]. Hence $\tilde{y} = (\hat{y} + I_k)B^*$, where $B^* := B^\dagger(BB^\dagger)^{-1}$. The resulting modified Riccati flow for $\hat{y}$ is

$$\hat{y}' = \hat{c} + \hat{d}\hat{y} - \hat{y}\hat{a} - \hat{y}\hat{b}\hat{y}.$$

where

$$\begin{aligned} \hat{c} &= \tilde{c}B + B^*\tilde{d}B - \tilde{a} - B^*\tilde{b}, \\ \hat{d} &= B^*\tilde{d}B - b^*\tilde{b}, \\ \hat{a} &= \tilde{a} + B^*\tilde{b}, \\ \hat{b} &= B^*\tilde{b}. \end{aligned}$$

Definition 1 (Matching function and condition). *We define the* determinantal matching function *to be* $\det \hat{y}(x;\lambda)$. *An isolated pure-point eigenvalue corresponds to the condition* $\det \hat{y}(+\infty;\lambda) = 0$.

1.4. Spectral shooting problem. In the context of the above, the goal in *spectral shooting* is as follows. Starting with the data $\hat{y}(-\infty;\lambda) := \tilde{y}(-\infty;\lambda)B(\lambda) - I_k$, we integrate forward with respect to x to compute $\hat{y}(+\infty;\lambda)$. Where the determinant of this square matrix is zero in Ω, corresponds to an isolated pure-point eigenvalue. Several issues immediately raise their head as follows:

(1) *Infinite integration range:* The integration range is infinite since $x \in \mathbb{R}$. We resolve this immediately using the 'tanh' transformation trick shown in Alexander, Gardner and Jones [**1**]. So from here-on, keeping this transformation in mind, and with our practical hats on, we will assume that our actual longitudinal domain is $x \in [-L, +L]$ for some large value $L > 0$.
(2) *Riccati singularities:* There are likely to be singularities in the modified Riccati flow for $\hat{y}$ as we integrate from $x = -L$ to $x = +L$. How can we account for these and do they have any special significance? Most of the rest of this manuscript is devoted to addressing this issue.
(3) *Further reduction:* Can we decompose the flow further? For example can we perform QR on $\hat{y}$ and follow the corresponding fibred flow?

2. Augmented unstable bundle

Let us adjust our perspective somewhat and align ourselves with the picture in Alexander, Gardner and Jones. For the region Ω in the complex plane to the right of the essential spectrum, a more general goal would be: for a given simple closed contour $K \in \Omega$, determine the number of zeros of the Evans function $D(\lambda)$ inside the coutour (assume that no zeros lie on the contour). Hence our domain is $(x, \lambda) \in [-L, L] \times K$; and integrating we can determine $Y^-(x;\lambda)$ throughout the domain. Actually we would like to think of this construction as a flow on a complex fibre bundle over the base space $\mathbb{S}^2$, the fibres of the bundle being $\mathrm{Gr}(n, k)$. Indeed, if K° denotes the subregion of Ω strictly inside K, the base space is

$$\mathcal{B} = \big(\{-L\} \times K^\circ\big) \cup \big([-L, L] \times K\big) \cup \big(\{+L\} \times K^\circ\big) \cong \mathbb{S}^2.$$

Associated with every point $(x, \lambda) \in \mathcal{B}$ we have a solution in $\mathrm{Gr}(n, k)$ to the linear spectral problem. Indeed this *generalized Gauss map* $G\colon \mathcal{B} \to \mathrm{Gr}(n, k)$ is given by

$$(x, \lambda) \mapsto \begin{cases} Y^-(-L;\lambda), & \text{if } x = -L,\ \lambda \in K^\circ, \\ Y^-(x;\lambda), & \text{if } x \in (-L, L),\ \lambda \in K, \\ Y^+(+L;\lambda), & \text{if } x = +L,\ \lambda \in K^\circ. \end{cases}$$

We have been deliberately rapid and loose with this construction and some care in the interpretation is required; see Alexander, Gardner and Jones [**1**] for more details. As you expect, $Y^-(x;\lambda)$ represents the k-dimensional subspace section at $x \in [-L, L)$ associated with the unstable subspace of $x = -L$, for each λ. On the other hand, $Y^+(+L;\lambda)$ represents the k-dimensional subspace section at $x = +L$ associated with the *unstable* subspace of $x = +L$.

Hence we have a fibre bundle $\mathcal{E} \to \mathcal{B}$ whose fibres are $\mathrm{Gr}(n, k)$. Details of how to pull this back to the universal subbundle can be found on p. 178 in Alexander, Gardner and Jones. Details of how to determine the first Chern number of this bundle over $\mathcal{B} \cong \mathbb{S}^2$, using the gluing or clutching map and the determinantal bundle can be found on p. 189. We want to come to the Chern characteristic classes from another angle; we begin to pursue this next.

3. Matching/intersecting

Consider our spectral problem $Y' = A(x;\lambda)\,Y$ on $[-L,+L]\times\Omega$. Pick a simple closed curve $K\subseteq\Omega$. Our task is to start with the initial data $\hat{y}(-L;\lambda) = \tilde{y}(-L;\lambda)B(\lambda)-I_k$. Then we integrate the modified Riccati equation forward with respect to x for each $\lambda\in K$. We thus compute $\hat{y}(x;\lambda)$ for all $(x,\lambda)\in(-L,L)\times K$. Then if there are no singularities in $\hat{y}(x;\lambda)$ for any $(x,\lambda)\in(-L,L)\times K$, we compute the image of $\det\hat{y}(+L;\lambda)$ for each $\lambda\in K$. The number of times this image winds round the origin counts the number of zeros of $\det\hat{y}(+L;\lambda)$ inside K, and thus the number of isolated pure-point eigenvalues inside K.

However in practice, in the integration process of the Riccati equation, a singularity may have crept inside K. This would of course affect the argument principle for the image of $\det\hat{y}(+L;\lambda)$. We can account for this though, as follows. With a slight abuse of notation let $\det\hat{y}(x;K)$ denote the section of the image of $\det\hat{y}(+L;\lambda)$ for each $x\in[-L,+L]$, as λ traces through K. If we compute and follow $\det\hat{y}(x;K)$ as x varies from $-L$ to $+L$ we can in principle detect if any isolated zeros or poles enter or leave $[-L,+L]\times K$. For the sake of argument, suppose that $\det\hat{y}(-L;K)$ does not contain any zeros or poles. If we thus count the isolated zeros and poles entering and leaving $(-L,+L]\times K$, we can work out the number of eigenvalues inside $[-L,+L]\times K$.

We come to the question of what a zero or singularity of $\det\hat{y}(x;\lambda)$ is, or maybe more precisely, how are they manifested through $\hat{y}$? Recall $\hat{y}:=\tilde{y}B(\lambda)-I_k$ and

$$\det\hat{y}(x;\lambda) = -\det\begin{pmatrix}-\hat{y}(x;\lambda) & \tilde{y}(x;\lambda)\\ O & I_{n-k}\end{pmatrix} = \det\begin{pmatrix}I_k & \tilde{y}(x;\lambda)\\ B(\lambda) & I_{n-k}\end{pmatrix}.$$

Hence if one or more components of $\hat{y}$ become singular then so do the corresponding components of $\tilde{y}$. Also if $\det\hat{y}$ becomes zero then the rows in the matching matrix (on the right) become linearly dependent. Let us examine zeros of $\det\hat{y}$ first. We now have two natural parallel perspectives for finding eigenvalues, we can look for:

(1) appropriate intersections of $\begin{pmatrix}I_k & \tilde{y}(x;\lambda)\end{pmatrix}$ with $\begin{pmatrix}B(\lambda) & I_{n-k}\end{pmatrix}$; or
(2) vanishing of the determinant $\det\hat{y}$.

Note that $\begin{pmatrix}I_k & \tilde{y}(x;\lambda)\end{pmatrix}$ lies in the top cell $\mathcal{C}_{\{1,\ldots,k\}}(\mathbb{E}'_\bullet)$ and corresponds to the variety $\mathcal{X}_0(\mathbb{E}'_\bullet)$. Also $\begin{pmatrix}B(\lambda) & I_{n-k}\end{pmatrix}$ lies in the top cell $\mathcal{C}_{\{1,\ldots,k\}}(\mathbb{E}_\bullet)$ with corresponding variety $\mathcal{X}_0(\mathbb{E}_\bullet)$. They both belong to the Schubert cycle σ_0. To compute the product $\sigma_0\cdot\sigma_0$ we need to compute the intersection between the varieties $\mathcal{X}_0(\mathbb{E}'_\bullet)$ and $\mathcal{X}_0(\mathbb{E}_\bullet)$. From Pieri's formula to compute this intersection, we need to fill the k by $(n-k)$ rectangle with the two partitions from each variety. In this case we get a completely empty k by $(n-k)$ rectangle, and the intersection is zero. Thus the only mechanism for there to be a non-zero intersection is if either $\begin{pmatrix}I_k & \tilde{y}(x;\lambda)\end{pmatrix}$ or $\begin{pmatrix}B(\lambda) & I_{n-k}\end{pmatrix}$ change into appropriate cycles—or at least enter appropriate cycles as x becomes large.

Some further remarks are, the:

(1) larger $n\times n$ determinants above are independent of the flags chosen.
(2) smaller $k\times k$ determinant is independent of the flags chosen.
(3) condition that $\det\hat{y}$ vanish is equivalent to demanding $f_{34}=0$; and this corresponds to the variety and thus cycle of co-dimension one, $\sigma_{0,1}$.

4. Schubert cycles or "states"

To motivate the use of Schubert cycles here we will use the special case of the Grassmannian $\mathrm{Gr}(4,2)$. Most of what we say generalizes to $\mathrm{Gr}(n,k)$ for any finite pair $k \leqslant n$. From the last section, we see that we are interested in mechanisms for cycle or *state* changes. Indeed if we are integrating $\hat{y}(x;\lambda)$ or equivalently $\tilde{y}(x;\lambda)$ there are two mechanisms that can instigate a cycle/state change:

(1) *Singular components:* If one or more components of $\hat{y}(x;\lambda)$ or $\tilde{y}(x;\lambda)$ become singular, then $\big(I_k \quad \tilde{y}(x;\lambda)\big)$ changes cell, variety and cycle.
(2) *Vanishing components:* If one or more components of $\hat{y}(x;\lambda)$ or $\tilde{y}(x;\lambda)$ become zero, then $\big(I_k \quad \tilde{y}(x;\lambda)\big)$ *may* change cell, variety and cycle.

4.1. Singular components. Let first consider an example in detail, before we enumerate all the possibilities for $\mathrm{Gr}(4,2)$. Suppose a 2-plane Y is in the top cell $\mathcal{C}_{\{1,2\}}(\mathbb{E}'_\bullet)$ in $\mathrm{Gr}(4,2)$ and thus given by

$$\begin{pmatrix} 1 & 0 & y_{11} & y_{12} \\ 0 & 1 & y_{21} & y_{22} \end{pmatrix}.$$

Let us suppose as we are integrating the Riccati equation governing y, and that one component appears to becoming large. Suppose that for $x = x^* - \epsilon$ with $0 < \epsilon \ll 1$ we appear to have the scaling $y_{11} \sim z_{11}/\epsilon$ as $\epsilon \to 0$. Here we suppose z_{11}, y_{12}, y_{21} and y_{22} are all *strictly of order unity* as $\epsilon \to 0$; see Hinch [**9**, p. 6]. Then a rank 2 transformation of the 2-plane Y to itself given by $\mathrm{diag}\{\epsilon, 1\}$, generates

$$\begin{pmatrix} \epsilon & 0 & z_{11} & \epsilon y_{12} \\ 0 & 1 & y_{21} & y_{22} \end{pmatrix} \to \begin{pmatrix} 0 & 0 & z_{11} & 0 \\ 0 & 1 & y_{21} & y_{22} \end{pmatrix},$$

as $\epsilon \to 0$. We perform three elementary row operations (eros). First we swap the rows; which is a rank 2 transformation generated by the matrix with zeros on the diagonal and ones off the diagonal. Second we normalize the z_{11} to one; this is achieved by a rank 2 transformation generated by $\mathrm{diag}\{1, z_{11}^{-1}\}$. This generates

$$\begin{pmatrix} 0 & 1 & y_{21} & y_{22} \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

Third we perform the elementary row operation consisting of the rank 2 transformation generated by the matrix

$$\begin{pmatrix} 1 & -y_{21} \\ 0 & 1 \end{pmatrix}$$

which generates

$$\begin{pmatrix} 0 & 1 & 0 & y_{22} \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

which lies in $\mathcal{C}_{\mathbf{j}}(\mathbb{E}'_\bullet)$ with $\mathbf{j} = \{2,3\}$. However, importantly one of the cell components is zero, and we might ask ourselves which cycle/state this solution is now in? Let $E_{ij} \in \mathrm{GL}(4)$ represent the elementary matrix constructed by swapping columns i and j of the matrix I_4; see Meyer [**13**, p. 131]. Then right multiplication of the matrix above by E_{34} generates

$$\begin{pmatrix} 0 & 1 & y_{22} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

which lies in $\mathcal{C}_{\mathbf{j}}(\mathbb{F}_\bullet)$ with $\mathbf{j} = \{2,4\}$. Here $\mathbb{F}_\bullet$ is the flag obtained from $\mathbb{E}'_\bullet$ by swapping the third and fourth ordinates. Since a Schubert cycle is invariant to

GL(n) translates, the varieties indicated by the last two matrices are in the same Schubert cycle or state, namely σ_μ with $\mu = \{1, 2\}$.

To be completely comprehensive, let us view the same situation in terms of Plücker coordinates. The procedure above, up to the rank 4 transformations, can be viewed as the following sequence of operations, starting with the Plücker embedding,

$$Y \mapsto \big\{f_{12}(Y), f_{13}(Y), f_{14}(Y), f_{23}(Y), f_{24}(Y), f_{34}(Y)\big\},$$

and finishing with the projection onto the Plücker quadrics. We get:

$$\begin{aligned}
\begin{pmatrix} 1 & 0 & z_{11}/\epsilon & y_{12} \\ 0 & 1 & y_{21} & y_{22} \end{pmatrix} &\mapsto \big\{1, y_{21}, y_{22}, -z_{11}/\epsilon, -y_{12}, z_{11}y_{22}/\epsilon - y_{12}y_{21}\big\} \\
&\xrightarrow{\text{scale}} \big\{\epsilon, \epsilon y_{21}, \epsilon y_{22}, -z_{11}, -\epsilon y_{12}, z_{11}y_{22} - \epsilon y_{12}y_{21}\big\} \\
&\xrightarrow{\epsilon\to 0} \big\{0, 0, 0, -z_{11}, 0, z_{11}y_{22}\big\} \\
&\xrightarrow{\text{normz}} \big\{0, 0, 0, 1, 0, -y_{22}\big\} \\
&\xrightarrow{\text{proj}} \begin{pmatrix} 0 & 1 & 0 & y_{22} \\ 0 & 0 & 1 & 0 \end{pmatrix}.
\end{aligned}$$

The final rank 4 transformation, swapping columns 3 and 4, reveals the Schubert cycle to be σ_{12}.

Now let us enumerate all the possibilities for $\mathrm{Gr}(n, k)$. Suppose a 2-plane Y is in the top cell $\mathcal{C}_{\{1,2\}}(\mathbb{E}'_\bullet)$ in $\mathrm{Gr}(4, 2)$ and thus given by

$$\begin{pmatrix} 1 & 0 & y_{11} & y_{12} \\ 0 & 1 & y_{21} & y_{22} \end{pmatrix}.$$

Again let us suppose we are integrating the Riccati equation governing y, and that one component appears to becoming large, in particular $y_{ij} \sim z_{ij}/\epsilon$ as $\epsilon \to 0$, with all the other remaining components and z_{ij} all *strictly of order unity* as $\epsilon \to 0$. Then a rank 2 transformations of the 2-plane Y to itself, followed by a GL(4) transformation taking $\mathbb{E}'_\bullet$ to another complete flag $\mathbb{F}_\bullet$, yields for $k \neq i$ and $\ell \neq j$:

$$\begin{pmatrix} 0 & 1 & y_{k\ell} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \in \sigma_{1,2}.$$

Now let us suppose any two pairs of the four possible components become singular as $\epsilon \to 0$. For the cases when y_{i1} and y_{i2} become singular, after a series of rank 2 transformations followed by a GL(4) transformation we get

$$\begin{pmatrix} 0 & 1 & 0 & * \\ 0 & 0 & 1 & * \end{pmatrix} \in \sigma_{1,1}.$$

For the cases when y_{ij} and y_{ji} become singular, after a series of rank 2 transformations followed by a GL(4) transformation we get

$$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \in \sigma_{0,0}.$$

This last case is also the result if any combination of three terms become singular simultaneously. The last case we have not considered is the case when y_{1j} and y_{2j} become singular simultaneously. In this case using the Plücker coordinates is more illuminating. Let us consider the case $j = 2$, the case $j = 1$ is analogous. Then as above, we see that

$$\begin{pmatrix} 1 & 0 & y_{11} & z_{12}/\epsilon \\ 0 & 1 & y_{21} & z_{22}/\epsilon \end{pmatrix} \mapsto \{1, y_{21}, z_{22}/epsilon, -y_{11}, -z_{12}/\epsilon, y_{11}z_{22}/\epsilon - z_{12}y_{21}/\epsilon\}$$

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$$\begin{aligned} &\xrightarrow{\text{scale}} \{\epsilon, \epsilon y_{21}, z_{22}, -\epsilon y_{11}, -z_{12}, y_{11}z_{22} - z_{12}y_{21}\} \\ &\xrightarrow{\epsilon\to 0} \{0, 0, z_{22}, 0, -z_{12}, y_{11}z_{22} - z_{12}y_{21}\} \\ &\xrightarrow{\text{normz}} \{0, 0, 1, 0, -z_{12}/z_{22}, y_{11} - z_{12}y_{21}/z_{22}\} \\ &\xrightarrow{\text{proj}} \begin{pmatrix} 1 & -z_{12}/z_{22} & y_{11} - z_{12}y_{21}/z_{22} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \end{aligned}$$

We see that this belongs to the Schubert cycle $\sigma_{0,2}$. One question we are left with is: can the cycle/state $\sigma_{0,1}$ be realized from the top cell through one or more components becoming singular? Or perhaps from a lower cell? Note that in all the cases above the GL(4) transformations involved were all products of matrices $E_{ij} \in \mathrm{GL}(4)$.

|| should be $\sigma_{0,2}$?

4.2. Vanishing components. As above, suppose that a 2-plane Y is in the top cell $\mathcal{C}_{\{1,2\}}(\mathbb{E}'_\bullet)$ in Gr(4, 2) and given by

$$\begin{pmatrix} 1 & 0 & y_{11} & y_{12} \\ 0 & 1 & y_{21} & y_{22} \end{pmatrix}.$$

Let us suppose as we are integrating the Riccati equation governing y, and that one or more components appear to become vanishingly small.

First let us consider the case that in Y, fleetingly, only one component, $y_{ij} \to 0$ as $\epsilon \to 0$. Then by a series of rank 2 transformations and rank 4 transformations of the form $E_{ij} \in \mathrm{GL}(4)$ generate

$$\begin{pmatrix} 1 & * & 0 & * \\ 0 & 0 & 1 & * \end{pmatrix} \in \sigma_{0,1}.$$

Now consider the case when y_{i1} and y_{i2} become zero, then after some transformations, we arrive at

$$\begin{pmatrix} 1 & * & * & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \in \sigma_{0,2}.$$

please ignore this part !

If y_{1j} and y_{2j} become zero, then after some transformations, we arrive at

$$\begin{pmatrix} 0 & 1 & 0 & * \\ 0 & 0 & 1 & * \end{pmatrix} \in \sigma_{1,1}.$$

If any three terms become simultaneously zero we will get

$$\begin{pmatrix} 0 & 1 & * & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \in \sigma_{1,2}.$$

We left the two trickiest cases to last. Consider the case $y_{11} \to 0$ and $y_{22} \to 0$ as $\epsilon \to 0$. First let us start in the top cell $\mathcal{C}_{1,2}(\mathbb{E}'_\bullet)$ and thus variety $\mathcal{X}_{0,0}(\mathbb{E}'_\bullet) = \{Y : f_{12} = 1\}$, and take $y_{11} \to 0$ so that we get

$$\begin{pmatrix} 1 & 0 & 0 & y_{12} \\ 0 & 1 & y_{21} & y_{22} \end{pmatrix}.$$

A row swap, which is a rank 2 transformation, followed by two column swaps, which are rank 4 transformations, generates

$$\begin{pmatrix} 1 & y_{21} & 0 & y_{22} \\ 0 & 0 & 1 & y_{12} \end{pmatrix}.$$

This lies in $\mathcal{X}_{0,1}(\mathbb{F}_\bullet)$ for some flag $\mathbb{F}_\bullet$. Indeed it is precisely $\mathcal{X}_{0,1}(\mathbb{F}_\bullet) = \{Y \in \mathrm{Gr}(4,2)\colon f_{12}(Y) = 0\}$. We see that $f_{34}(Y) \equiv y_{22}$. Further recall the Plücker relation $f_{12}f_{34} - f_{13}f_{24} + f_{14}f_{23} = 0$. We see that setting $y_{22} = 0$ does not change the cell or variety. A similar argument applies to the case $y_{12} \to 0$ and $y_{21} \to 0$.

Hence we conclude that, as we integrate $\hat{y}$, components becoming singular necessarily precipitate a change of cycle/state, while components becoming zero, might do so.

5. Stability of parabolic travelling waves

5.1. Parabolic systems. We start with some general remarks about computing the stability of travelling wave solutions to semilinear parabolic partial differential equations. Consider the parabolic system:

$$\partial_t U = D\,\partial_{xx} U - \bar{c}\,\partial_x U + F(U),$$

where D is a diagonal matrix of positive diffusion coefficients. We suppose we are in a frame of reference travelling to the right with speed $\bar{c}$, which coincides with the speed of the travelling waves whose stability we wish to study. Linearizing about the travelling wave $\bar{U}(x)$, the stability problem expressed in the form $Y' = A(x;\lambda)\,Y$ has coefficient matrix

$$A(x;\lambda) = \begin{pmatrix} O & I \\ D^{-1}\big(\lambda I - \mathrm{d}F(\bar{U})\big) & -\bar{c}\,D^{-1} \end{pmatrix}.$$

In this coefficient matrix, denote the top left, right and lower left, right blocks a, b, c and d. We notice that $a = O$ and $b = I$ in particular, and that the only non-autonomous block is $c = c(x)$. If we write down the Riccati flow in the top cell of the Grassmannian we would have

$$y' = c(x) + dy - y^2.$$

Since $d = -\bar{c}\,D^{-1}$ is constant we can always rescale y to obtain a modified Riccati equation similar to that above with the linear term missing. Rather nicely, the non-autonomous part $c(x)$ is present as a purely additive non-homogeneous term; and therein lies all the essential structural-determining information.

5.2. Autocatalytic waves. We study travelling waves in a model of autocatalysis in an infinitely extended medium

$$\begin{aligned} u_t &= \delta u_{xx} + \bar{c}\,u_x - uv^m, \\ v_t &= v_{xx} + \bar{c}\,v_x + uv^m. \end{aligned}$$

Here $u(x,t)$ is the concentration of the reactant and $v(x,t)$ is the concentration of the autocatalyst. We suppose (u,v) approaches the stable homogeneous steady state $(0,1)$ as $x \to -\infty$, and the unstable homogeneous steady state $(1,0)$ as $x \to +\infty$. The diffusion parameter δ is the ratio of the diffusivity of the reactant to that of the autocatalyst and m is the order of the autocatalytic reaction. The speed of the co-moving reference frame is $\bar{c}$. The system is globally well-posed for smooth initial data and any finite $\delta > 0$ and $m \geqslant 1$. We know that a unique heteroclinic connection between the unstable and stable homogeneous steady states exists for wavespeeds $\bar{c} \geqslant c_{\min}$. The unique travelling wave for $\bar{c} = c_{\min}$ converges exponentially to the homogeneous steady states and is computed by a simple shooting algorithm. The stability of the travelling wave of velocity $\bar{c}$ can be deduced from the location of the spectrum of the eigenvalue problem $Y' = A(x;\lambda)Y$, where

$$A(x;\lambda) = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \lambda/\delta + \bar{v}^m/\delta & m\bar{u}\bar{v}^{m-1}/\delta & -\bar{c}/\delta & 0 \\ -\bar{v}^m & \lambda - m\bar{u}\bar{v}^{m-1} & 0 & -\bar{c} \end{pmatrix},$$

where $\bar{u}$ and $\bar{v}$ represent the travelling wave solution. The pulsating instability occurs when $\delta < 1$ is sufficiently small and m is sufficiently large. For δ fixed and m increasing, a complex conjugate pair of eigenvalues crosses into the right-half λ-plane signifying the onset of instability via a Hopf bifurcation.

5.3. Grassmannian. For this problem the Grassmannian is $\mathrm{Gr}(4,2)$ and we define the Evans function slightly differently than above. In the coefficient matrix $A(x;\lambda)$ above denote the top left, right and lower left, right blocks a, b, c and d. The matching condition is

$$\det\begin{pmatrix} I_2 & I_2 \\ y(x;\lambda) & B(\lambda) \end{pmatrix} = -\det\big(\hat{y}\big) = 0$$

where $\hat{y} := y - B(\lambda)$ and $B(\lambda) := y^+(+\infty;\lambda)$. The modified Riccati flow for $\hat{y}$ is

$$\hat{y}' = \hat{c} + \hat{d}\hat{y} - \hat{y}\hat{a} - \hat{y}b\hat{y}.$$

where

$$\begin{aligned} \hat{c} &= c + dB - Ba - BbB, \\ \hat{d} &= d - Bb, \\ \hat{a} &= a + bB. \end{aligned}$$

Note that $B(\lambda) = y^+(+\infty;\lambda)$ is in fact stationary solution of the modified Riccati flow for large x, hence we have that

$$\lim_{x\to\infty} \hat{c} = 0.$$

Further note that for the autocatalytic problem, $a = 0$ and $d = -\bar{c}\,\mathrm{diag}\{\delta^{-1}, 1\}$. Explicitly,

$$B(\lambda) = -\tfrac{1}{2}\begin{pmatrix} \big(\bar{c} + \sqrt{\bar{c}^2 + 4\delta\lambda}\big)/\delta & 0 \\ 0 & \bar{c} + \sqrt{\bar{c}^2 + 4\lambda} \end{pmatrix}.$$

5.4. Far-field behaviour. By the far-field behaviour, we mean the behaviour of the solutions to the Riccati equation for $\hat{y}$ above as $x \to +\infty$. Note that for large x the Riccati system has the following form (recall $\hat{c}(x) \to 0$ as $x \to +\infty$):

$$\hat{y}' = (d - B)\hat{y} - \hat{y}B - \hat{y}^2.$$

Indeed, using that d and B are diagonal matrices we get, explicitly:

$$\begin{aligned}
y_{11}' &= (d_1 - B_1)y_{11} - B_1 y_{11} - y_{11}^2 - y_{12}y_{21},\\
y_{12}' &= (d_1 - B_1)y_{12} - B_2 y_{12} - (y_{11} + y_{22})y_{12},\\
y_{21}' &= (d_2 - B_2)y_{21} - B_1 y_{21} - (y_{11} + y_{22})y_{21},\\
y_{22}' &= (d_2 - B_2)y_{22} - B_2 y_{22} - y_{22}^2 - y_{12}y_{21}.
\end{aligned}$$

We know from Schneider [**17**, Theorem 2'] that this autonomous Riccati system has a unique sink as $x \to +\infty$. In other words, for each λ, there is a unique asymptotic state $\hat{y}_+(\lambda)$ as $x \to +\infty$.

5.5. Far-field stationary solutions. If we look for stationary solutions to the modified Riccati flow as $x \to +\infty$ we arrive at the algebraic system of equations:

$$(d - B)\hat{y} - \hat{y}B - \hat{y}^2 = 0,$$

or, componentwise,

$$\begin{aligned}
(d_1 - 2B_1)y_{11} - y_{11}^2 - y_{12}y_{21} &= 0,\\
y_{12}(d_1 - B_1 - B_2 - y_{11} - y_{22}) &= 0,\\
y_{21}(d_2 - B_2 - B_1 - y_{11} - y_{22}) &= 0,\\
(d_2 - 2B_2)y_{22} - y_{22}^2 - y_{12}y_{21} &= 0.
\end{aligned}$$

Explicitly, collecting results for the diagonal matrices d and B from above,

$$\begin{aligned}
B_1 &= -\tfrac{1}{2}\big(\bar{c} + \sqrt{\bar{c}^2 + 4\delta\lambda}\big)/\delta,\\
B_2 &= -\tfrac{1}{2}\big(\bar{c} + \sqrt{\bar{c}^2 + 4\lambda}\big),\\
d_1 - B_1 &= \tfrac{1}{2}\big(-\bar{c} + \sqrt{\bar{c}^2 + 4\delta\lambda}\big)/\delta,\\
d_2 - B_2 &= \tfrac{1}{2}\big(-\bar{c} + \sqrt{\bar{c}^2 + 4\lambda}\big).
\end{aligned}$$

5.6. Simulations and observations. For values of $\lambda \in \Omega$ we integrated the Riccati system for $\hat{y}$ from $x = -L$ to $x = +L$. In Figures 1 and 2 we plotted the Riccati solution components for four significant λ values ($\lambda = 0$ is naturally an eigenvalue).

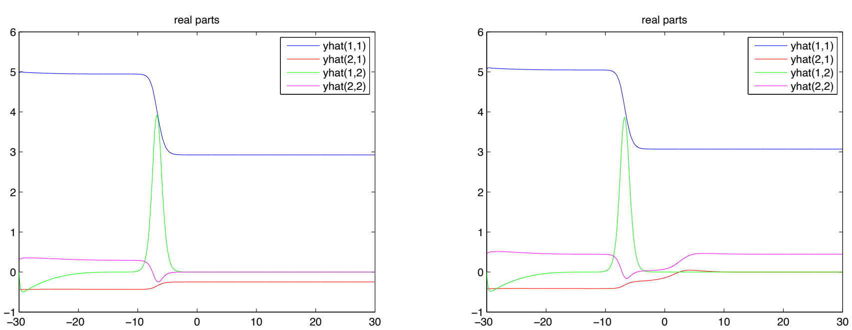

FIGURE 1. Entries $\hat{y}$ for (left) $\lambda = 0$ (right) $\lambda \neq$ eigenvalue.

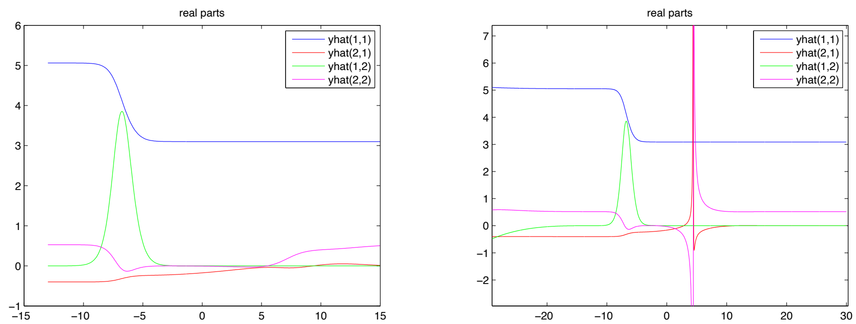

FIGURE 2. Entries $\hat{y}$ for (left) λ close to the eigenvalue (right) singularity.

In Figure 3 we considered values of λ in the top right quadrant as shown. For each value of λ we integrated the Riccati system for $\hat{y}$ from $x = -L$ to $x = +L$. As integration proceeded, for most values of λ, the solution components of $\hat{y}(x)$ all remained bounded for all $x \in [-L, +L]$. However for some values of lambda, at one value $x_\star \in [-L, +L]$, some components of $\hat{y}(x)$ became singular. In particular, in the three-space $[-L, +L] \times \overline{K^\circ}$ where $\overline{K^\circ}$ is the λ-quadrant shown, there is a one-dimensional curve where some components of $\hat{y}(x)$ become singular. This *singularity locus* spirals into the eigenvalue as $x \to \infty$. We show in Figure 3 the projection of this singularity locus onto $\{+L\} \times \overline{K^\circ}$. If we were to perform an analogous plot for when $\det \hat{y}$ is small there would be a similar one-dimensional *zero locus* curve in $[-L, +L] \times \overline{K^\circ}$ converging towards the eigenvalues as $x \to \infty$; except that it does not spiral as much singularity locus.

|| λ

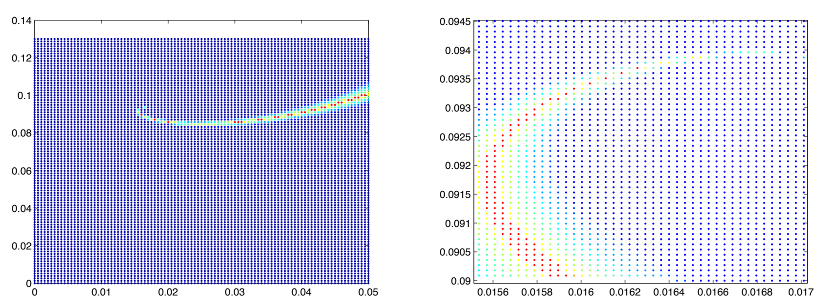

FIGURE 3. Maximum value in $\hat{y}$ from dark blue (< 5) to red (singularity). The X-axis shows the real part of λ, the Y-axis is the imaginary part. The red stars/dots appear for those λ-values where $\hat{y}$ became infinite in the matlab-code (possibly some red stars/dots do not represent a singularity but really large values near the singularity: values $> 2^{1024}$ give infinite values in matlab). The pink star appears where the Evans function $\det \hat{y}$ is minimal (=eigenvalue), at the tip of the red curve. There is a singular one-dimensional curve in $(-L, L) \times \overline{K^\circ}$ that spirals into the eigenvalue. What is shown is the projection onto $\{+L\} \times \overline{K^\circ}$.

Our first *important observation*, yet to be proved analytically, is that for all λ in the quadrant shown, $y_{12}(x;\lambda) \to 0$ as $x \to +\infty$. If we substitute this fact into the system of quadratic algebraic equations for the far-field stationary solutions above, then assuming that y_{11} and y_{22} are non-zero, we deduce that $y_{21} = 0$ and $y_{11} = d_1 - 2B_1$ and $y_{22} = d_2 - 2B_2$. These values match with all the final values for these components with one exception; we assume this represents the unique sink solution for $x \to +\infty$. The exception is of course the eigenvalue. For the eigenvalue, since $\det \hat{y}(+L;\lambda) = 0$, we believe the far-field ansatz for the *eigenfunction* to be

$$\hat{y}(x;\lambda) \sim \begin{pmatrix} d_1 - 2B_1 & 0 \\ y_{21} & 0 \end{pmatrix},$$

as $x \to +\infty$. Direct substitution into the modified Riccati equation as $x \to +\infty$ yields that for some constant $\tilde{C}_0 \neq 0$,

$$y_{21} = \tilde{C}_0 \exp\big((d_2 - B_2 - d_1 + B_1)\,x\big).$$

A second set of *important observations* concerning the nature of the singularities are noteworthy. Firstly, y_{11} and y_{12} are never singular. The singularites in y_{21} and y_{22} only appear once the travelling front has been traversed; in fact well beyond that juncture. Since for large x we observe $y_{12} \approx 0$, we can deduce that the far-field equation governing y_{22} decouples from the other components and satisfies

$$y_{22}' = (d_2 - 2B_2)y_{22} - y_{22}^2.$$

If, once past the travelling front, y_{22} becomes negative, then it must become singular—this could potentially be used as an eigenvalue determining criterion. Indeed, the singularity is a simple pole with repsect to x. Looking at the analogous equation for y_{21} for large x, we soon see that ~~that~~ must also have a simple pole simultaneously.

A third *important observation* combines the last two. Recall the discussion in Section 4 on Schubert cycles. Note that the asymptotic ansatz for the eigensolution means that it belongs to the Schubert cycle $\sigma_{0,2}$. On the other hand, the singular ansatz just described drops us from the top cycle $\sigma_{0,0}$ into the cycle $\sigma_{0,2}$! Hence we conjecture the following.

CONJECTURE 1. *The* singular *and* zero loci *are the same curve, perhaps the same closed curve, closed off at "infinity". If λ^* is the eigenvalue, we do know they meet at $\{+L\} \times \{\lambda^*\}$, the question is how they closed off in the left-half λ-plane.*

6. Sphere punctures

In this section we are extremely speculative. We state goals/scenarios we would like to see.

(1) Dissecting the spectral space: Do the loci of cycle changes determine the whole spectral space $[-L, L] \times \Omega$?
(2) Cohomology of the spectral space: Another way to view this last statement, do the loci dissect the spectral space into closed sets, such that each point inside is homotopic to the characteristic state identifying the closed set?
(3) Punctures of the spectral sphere: since the base space $\mathcal{B} \cong \mathbb{S}^2$, all we need to do, is to look for where the lower dimensional cycle loci puncture the sphere and count the total?

(4) Reparameterizing the spectral sphere: can we reparameterise the spectral sphere and coordinatize it in a favourable way in order to efficiently locate these subcycle punctures?

Let us try to address these with the following comments, suggestions and observations.

> So singular and zero loci curves of $\det \hat{y}(x;\lambda)$ are the same Schubert cycle; they indicate an eigenvalue if they meet at $x = +\infty$. For the autocatalytic problem for the physical parameters chosen, there's one loci curve in the upper λ-plane and one in the lower. Indeed even these may be connected. In any case, let us suppose we are considering a parabolic problem for which the linear stability operator is *sectorial*. Let $\overline{K^\circ}$ denote the minimal subset of the upper-right λ-quadrant containing the upper half of the sector where the spectrum may lie—the finite subregion that includes intervals of the real and imaginary axes starting at the origin.
>
> For the three-space $[-L, +L] \times \overline{K^\circ} \cong \mathbb{D}^3$, we know a loci curve enters across the imaginary axis for some value $x = x_*$. Let us follow that curve as x increases to $+\infty$. It will lead us to an eigenvalue. Denote the loci curve in $\mathbb{D}^3$ by $\ell = \ell(x,\lambda)$. The whole of the space $\mathbb{D}^3 \backslash \ell$ is homotopic to the trivial state. We can ignore it.
>
> Hence here is a suggested numerical procedure. Integrate the modified Riccati equation for values of λ on the imaginary axis, within the sectorial interval. Scan for when a loci punctures/crosses the axis. Follow the curve corresponding to ℓ ignoring everything else; for the autocatalysis problem this means follow the curve given by the state/cycle $\sigma_{0,2}$.
>
> The question: is this possible? How can we follow such a curve? Does this give a more efficient way to determine *instability*?

References

[1] Alexander, J.C., Gardner, R. and Jones, C.K.R.T.: A topological invariant arising in the stability analysis of traveling waves. J. Reine Angew. Math. 410, 167–212 (1990)

[2] Billey, S.: Introduction to affine Grassmannians. talk, January 23, 2009

[3] Chern, S.S.: Complex manifolds without potential theory. Van Nostrand Mathematical Studies #15, (1967)

[4] Coskun, I.: Grassmannians: the first example of a moduli space. MITOpenCourseWare available at `http://ocw.mit.edu/NR/rdonlyres/Mathematics/18-727Spring-2006`

[5] Fulton, W.: Young tableaux. London Mathematical Society Student Texts 35, Cambridge University Press, (1997)

[6] Griffiths, P. and Harris, J.: Principles of algebraic geometry. Wiley Classics Library Edition, (1994)

[7] Hatcher, A.: Algebraic topology. Cambridge University Press, (2002), available to download from `http://www.math.cornell.edu/~hatcher`

[8] Hatcher, A.: Vector bundles and K-theory. (2003), `http://www.math.cornell.edu/~hatcher`

[9] Hinch, E.J.: Perturbation methods. Cambridge Texts in Applied Mathematics, Cambridge University Press, (1991)

[10] Kleiman, S.L. and Laksov, D.: Schubert calculus. The American Mathematical Monthly 79(10), 1061–1082 (1972)

[11] Kresch, A.: Flag varieties and Schubert calculus. preprint, July 2005
[12] Ledoux, V., Malham, S.J.A. and Thümmler, V.: Grassmannian spectral shooting. Accepted Math. Comp., (2008)
[13] Meyer, C.: Matrix analysis and applied linear algebra. SIAM (2000)
[14] Milnor, J.W. and Stasheff, J.D.: Characteristic classes. Annals of mathematics studies 76, Princeton University Press, (1974)
[15] Montgomery, R.: A tour of subRiemannian geometries, their geodesics and applications. Mathematical Surveys and Monographs 91, American Mathematical Society, (2002)
[16] Postnikov, A.: Total positivity, Grassmannians, and Networks. arXiv:math/060976v1 27 Sep 2006
[17] Schneider, C.R.: Global aspects of the matrix Riccati equation. Theory of Computing Systems 7(3), 281–286 (1973)
[18] Shayman, M.A.: Phase portrait of the matrix Riccati equation. SIAM J. Control Optim. 24(1), 1–65 (1986)
[19] Sottile, F.: Rational curves on Grassmannians: systems theory, reality, and transversality. In "Advances in Algebraic Geometry Motivated by Physics", ed. by Emma Previato, Contemporary Mathematics 276, 9–42 (2001)
[20] Steenrod, N.: The topology of fibre bundles. Princeton University Press, (1951)
[21] Warner, F.W.: Foundations of differentiable manifolds and Lie groups. Graduate texts in mathematics, Springer, (1983)

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These notes are a summary write of work completed during the summer of 2009. For one month in that summer Veerle Ledoux came to visit SJAM at Heriot-Watt. Our goal had been to try to make the direct connection between singularities in the Riccati equation which seemed to converge to eigenvalues in the far field limit, that Veerle had observed numerically. We explored a lot of analytical and numerical avenues. Indeed Veerle completed vast amounts of numerical work and simulations that are not included above (she has them recorded somewhere). The analytical avenues are mainly what is recorded here. And as we were quite new to all the required algebraic geometry, some naivety in our analysis should be forgiven on the part of the reader. We've tried to indicate which parts should be ignored (because they're essentially not correct---with hindsight and now more understanding). However we refer to this manuscript in other papers quite a bit as it is the first place where we first properly wrote down the Riccati singularity and eigenvalues connection result in some form of manuscript (together with a lot of open ended avenues, conjectures and musings). So please treat with care, though at the same time enjoy some (sometimes way-out) ideas/suggestions....

Simon Malham 21/8/2014